

Discrete Spectrum in Bose Condensation

Enrico Celeghini¹ and Mario Rasetti²

¹ *Dipartimento di Fisica, and Sezione INFN,
Università di Firenze, I-50125 Firenze, Italy*

² *Dipartimento di Fisica, and Unità INFN,
Politecnico di Torino, I-10129 Torino, Italy*

A quantitative description of the whole process of condensation of bosons in an harmonic trap is given resorting only to Gibbs and Bose postulates, without assuming equipartition nor continuum statistics. Below T_c discrete spectrum theory predicts for the thermo-dynamical variables a behavior different from the continuum case. In particular a new critical temperature T_d is found where the specific heat exhibits a λ -like spike. Numerical values of the relevant quantities depend on the experimental set-up. The theory does not take into account collective effects in the ground state.

PACS numbers: 03.75.Fi, 05.30.Jp

Bose-Einstein condensation (BEC) was discovered (or, better, predicted) by Bose [1] and Einstein [2] in 1924-25 studying the properties of a gas of non interacting bosons in a (infinite) box. BEC has been experimentally observed only in 1995, in vapors of rubidium [3] and sodium [4] confined in magnetic traps and cooled. Present research on BEC follows similar experimental lines, where the potential makes the spectrum discrete [5], [6]. Theoretical research on BEC in traps is also in tumultuous progress [7], focusing essentially on the role of interactions among the atoms. Here we shall instead pay attention more to the relation between the discreteness and multiplicity of the quantum mechanical spectrum, and the features induced by quantum statistics.

BEC in a box (where the walls do not essentially affect the continuity of the spectrum) and BEC in an harmonic trap (whose effect is to make the spectrum definitely discrete), coincide only in some approximate way. First of all, in a magnetic trap the number N of confined particles as well as the volume V in which they are confined are finite, namely we are not in the thermodynamic limit. This effect has been discussed in different papers [8], [9], [10], [11] and shown to have limited phenomenological relevance, as in the experiments the number of particles is $10^5 \div 10^7$. There is however another reason why the thermodynamic limit is not reached – and cannot be reached – in magnetic traps, on which we focus our attention here: the energy spectrum. Quantizing in a box, the difference between contiguous energy levels goes to zero at least as $V^{-1/3}$ as volume increases. On the other hand, in order to obtain the thermodynamic limit in an harmonic potential we should have to require that the oscillator frequency – i.e. the spacing of the spectrum – goes to zero as $N^{-1/3}$. One needs, in other words, that the spectrum may be considered continuous. This is far from the experimental situation, where typically $h\nu/k_B \approx 10 nK$ (for $\nu \approx 10^2 Hz$), to be compared with the estimated temperature $T_c \approx 10^2 nK$.

We shall attempt here to propose a better framework

within which experimental results are consistently described, trying to represent more properly BEC experimental situation (N finite, energy discrete). Even though keeping spectral structure into account may be an important step forward with respect to the continuum theory, many body effects are still not considered. The results are thus correct up to the detailed structure e.g. of the ground state, as it could be described by a collective perturbation in the space of free bosons, as in Gross-Pitaevsky approach [5], [7].

Ever since 1907 Einstein himself [12] had pointed out how classical results on equipartition of energy are no longer valid for $T < h\nu/k_B$ for the quantized harmonic oscillator in the frame of Boltzmann statistics. This has been so far disregarded, in spite also of the change in statistics, as $T < h\nu/k_B$ is below the range of experiments. Several other authors have on the other hand discussed BEC in the context of the present experimental situation using equipartition together with the continuum statistics (eq. (2) below) [13], [14], [15], finding that the temperature scale of the process is $\propto N^{1/3}$. Within the approach presented here this scaling law, essential for the coherence of the scheme, is recovered, among other novel results. The crucial difference is however that it is obtained by re-deriving the entire theory of bosons with discrete spectrum, based only on the Gibbs and Bose postulates. The central results are that a new equation (eq. (5) below) replaces the continuum distribution function, equipartition is valid only for $T > T_c$, and a new critical temperature is found.

Our motivation for this construction is the recent definition of bosons as coherent states of the algebra $su(1, 1)$, given in [16]. In that paper a possible generalization of the Bose definition of bosons has been considered. Here this is used only to define the undegenerate states of the harmonic oscillator as the limit for $g \rightarrow 1$ of the general formula (eq. (1) below).

We begin by summarizing the most relevant results that a thorough numerical analysis performed within this

conceptual scheme leads to, leaving for the second part of the paper some clarifying details. There turn out to be seven essential features when comparing the continuum and discrete cases:

1) The formula (eq. (5) below) for the occupation number $n(\epsilon_i)$ as a function of the single particle discrete energy ϵ_i is the same as in the thermodynamic limit at zero energy, moreover for discrete spectrum it does not decrease exponentially as $\epsilon \rightarrow \infty$ but rather it becomes identically zero for $\epsilon > \epsilon_{max}$ (where ϵ_{max} has a well defined value much less than the total energy E and goes to infinity only in the continuum limit). Measurable effects are related with the product of $n(\epsilon_i)$ with the multiplicity of energy levels $m(\epsilon_i)$. Fig. 1 displays the product $n(\epsilon_i)m(\epsilon_i)$ vs. i .

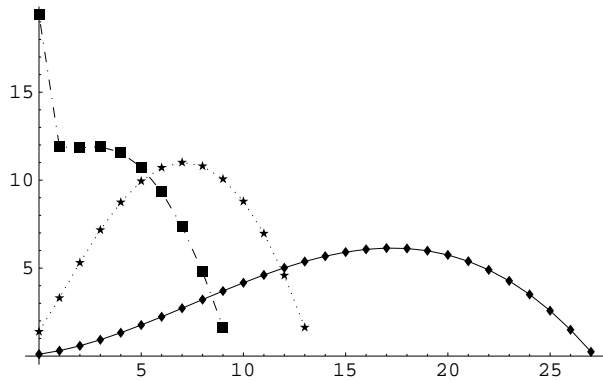


FIG. 1. $n(\epsilon_i)m(\epsilon_i)$ vs. i for $N = 10^2$ bosons in an isotropic harmonic trap for different values of T ($T_{\blacksquare} < T_{\star} < T_{\blacklozenge}$) in proximity of T_c , showing the appearance of $n_0 \neq 0$.

2) The Lagrange multiplier β' , that in the continuum is identically equal to $1/(k_B T)$ – and $\propto (E/N)^{-1}$ due to equipartition – is now for $T > T_c$ $\beta' \propto (E/N)^{-4}$, yet the equipartition theorem is still satisfied (constant specific heat). In other words, the Lagrange multiplier turns out to be a more complicated function of T than $\propto T^{-1}$.

3) Temperature, defined – without resorting to equipartition – as the derivative of energy with respect to entropy, allows us to describe entirely the thermodynamics of the system, assumed in global thermal equilibrium (as done in [13]) because of the efficiency of evaporative cooling. For $T \geq T_c$, effects related to the spectrum discreteness appear to be irrelevant, as they are in determining T_c as a function of N [14], [15]. Another critical temperature T_d is however found (see Fig. 2) defined by the ground state filling n_0/N crossing the value $1/2$.

As Fig. 2 shows, C is constant, equal to $3k_B$ (as it should, since the system does not condense and behaves as a classical gas) for $T > T_c$; it is almost zero (as entropy and energy decrease with quite different slopes because only a few atoms progressively migrate from the warmer tail of the spectrum into the fundamental level) for $T_d < T < T_c$, and exhibits a peak for $T = T_d$, where

condensation becomes a global effect. Note that, after the spike at T_d , the specific heat goes to zero as T goes to zero, as required by Nernst's theorem.

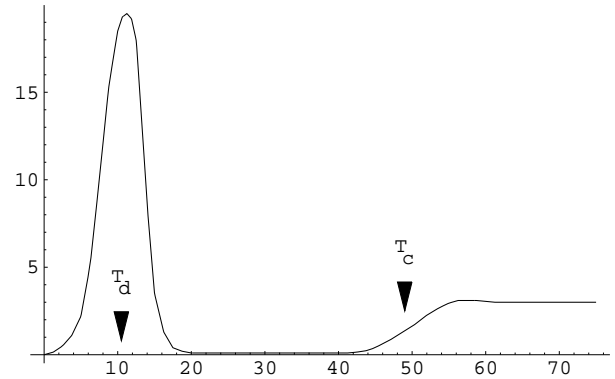


FIG. 2. Specific heat C vs. T in units $k_B = h\nu = 1$ for $N = 10^6$ bosons in an isotropic harmonic trap, as predicted by discrete quantum statistics.

4) The chemical potential is no longer equal to the Lagrange multiplier α' and does not appear to present major differences from the results reported in the literature [8].

5) Repeated numerical analysis for various values of N indicates that $T_c \propto N^{1/3}$, in agreement with [14], [15], whereas one finds $T_d \propto N^{1/3}/\ln N$.

6) As explicitly shown in Fig. 1, the high energy tail of the velocity distribution is not of Maxwell-Boltzmann type and it cannot be straightforwardly used to determine the experiment temperature [13].

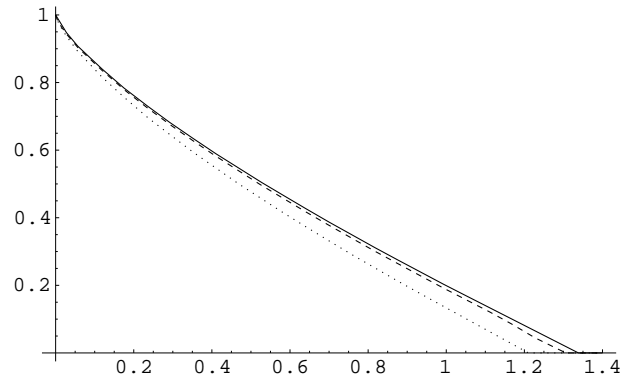


FIG. 3. The fraction of condensate n_0/N vs. $N^{-1/3} (E/Nh\nu - 3/2)$ for $N = 10^4$ (\cdots), 10^6 ($- - -$), 10^8 ($—$).

7) Thermo-dynamical temperature, despite its conceptual relevance, does not appear to be the physical parameter that best describes the process of condensation: it is difficult to measure in the typical experimental set-up, and as one does not have equipartition its intuitive meaning of "average energy per particle" is lost. We prefer then to describe the onset of condensation by exhibiting the behavior of n_0/N vs. the true (dimensionless)

"energy per particle" $E/Nh\nu$ (Fig. 3, where in abscissa we actually reported $N^{-1/3}(E/Nh\nu - 3/2)$ to point out the dependence on $N^{1/3}$), much easier to compare with experiments. Our results are consistent with the experimental findings in ref. [13]. Fig. 4, of which Fig. 2 shows the derivative, provides E/N as a function of T . This curve can be inverted giving $T = T(E/N)$, a relation which replaces equipartition (where it would be linear) and allows us to evaluate temperature dependent quantities as functions of the experimentally more accessible internal energy.

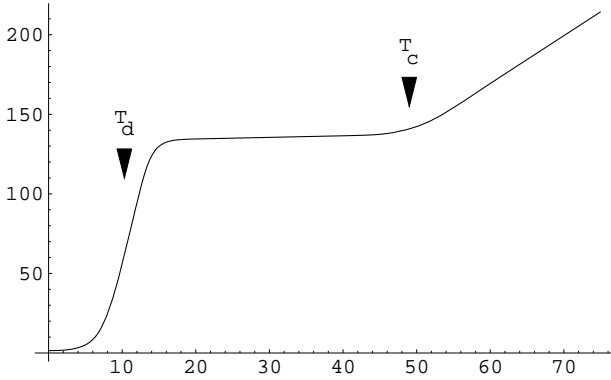


FIG. 4. Specific internal energy E/N vs. T , for $N = 10^6$ (units as in Fig. 2).

We shall now discuss in some mathematical detail how the above features come into play. The traditional textbook way (see e.g. [17]) of deriving the boson gas equilibrium distribution is the following. Starting from Gibbs' assumption, in order to derive the combinatorics many single particle states (levels) of energy practically equal are collected together in cells (an assumption justified *a posteriori* by the thermodynamic limit) and the particle distribution is straightforwardly found to be, up to normalization, given by

$$W\{n_i\} = \prod_i \frac{\Gamma(n_i + g)}{\Gamma(n_i + 1)\Gamma(g)},$$

where g is the multiplicity, that with no loss of generality we assume equal for all cells. The equilibrium distribution, identified with that of maximum probability, is then obtained by finding the set $\{n_i\}$ that maximizes (the logarithm of) $W\{n_i\}$, constrained by the two conditions $\sum_i n_i = N$ and $\sum_i \epsilon_i n_i = E$. One obtains the exact equation

$$\psi(n_i + g) - \psi(n_i + 1) = \alpha + \beta \epsilon_i \equiv h_i, \quad (1)$$

where $\alpha = \alpha(g)$, dimensionless, and $\beta = \beta(g)$, with the physical dimension of an inverse energy, are the two Lagrange multipliers, clearly depending on the value of g , introduced in order to implement the constraints, while ψ is the digamma function [18].

For large argument ψ coincides with the logarithm, thus for $n_i \gg 1$ and $g \gg 1$ it is easy to obtain (identifying $n(\epsilon_i)$ with the finite density n_i/g)

$$n(\epsilon_i) = \frac{1}{e^{h_i} - 1}. \quad (2)$$

The latter is the Bose-Einstein distribution we are accustomed to, so well established that it is sometimes considered as an alternative definition of bosons. The essential assumption of this derivation is of course that the energy spectrum is continuous, hypothesis that does not hold in the presence of an harmonic potential.

Eq. (1) has more general validity in that it holds true for any value of g and hence also for the discrete case. For example, in the case of photons in a laser beam, where degeneracy of states is two because of helicity, it gives [18]

$$n_i = \frac{1}{h_i} - 1 \text{ for } h_i < 1 \quad \text{and} \quad n_i = 0 \text{ for } h_i > 1. \quad (3)$$

For a physical (3-dimensional) quantum harmonic oscillator, g should be set equal to 1. Indeed, even in the "isotropic" case, that we shall consider as an example, the experimental frequencies are such that $\nu_i - \nu_j \ll \nu_i$, but ν_i is never exactly equal to ν_j ; we have then a computing degeneracy only, because statistics remains un-degenerate. However, setting $g = 1$ leads for (1) to a perfectly acceptable but void equation (left hand side identically zero, implying $\alpha(1) = \beta(1) = 0$). On the other hand: i) eq. (1) is defined for g in the whole complex plane except for negative integers, and ii) in ref. [16] an alternative definition of bosons has been proposed in terms of coherent states of the discrete series of $SU(1, 1)$, where the highest weight of the representation is $g/2$, with g any strictly positive real number. In this latter context g is not restricted to the integer values imposed by the combinatorial interpretation and we can define by analytical continuation for $g \rightarrow 1$ the equation for un-degenerate levels that we need. $n_i \equiv n(\epsilon_i)$ results thus to be the solution to the equation

$$\psi'(n_i + 1) = \alpha' + \beta' \epsilon_i \equiv h'_i, \quad (4)$$

where $\alpha' \equiv \lim_{g \rightarrow 1} \alpha(g)/(g - 1)$ and $\beta' \equiv \lim_{g \rightarrow 1} \beta(g)/(g - 1)$ are the new Lagrange multipliers to be determined by the constraints of fixed N and E , and ψ' is the trigamma function [18], derivative of ψ . Eq.(4) is one-to-one and can be inverted, giving us the correct formula for discrete spectrum, to be used instead of eq.(2):

$$n_i = [\psi']^{-1}(h'_i) - 1 \quad \text{for } h'_i < \pi^2/6 \quad (5)$$

and

$$n_i = 0 \quad \text{for } h'_i \geq \pi^2/6,$$

$[\psi']^{-1}$ denoting the inverse function of ψ' . $\pi^2/6 \equiv \psi'(1)$. For $h' \rightarrow 0$ eq. (5) has the same asymptotic behavior as

(2) : $n_i \rightarrow h'^{-1} - \frac{1}{2}$. The two formulas (2) and (5) exhibit a similar structure, characteristic of all values of g , with a pole (with residue 1) at argument zero and a zero for large values of the argument (compare eq. (3)). The discrete description, however, does not require an *ad hoc* delta function at the ground state, which is instead discussed on the same footing as all the others. In fact one may assign first the values of N and E ; from these the two Lagrange multipliers $\alpha' = \alpha'(N, E)$, $\beta' = \beta'(N, E)$ are then obtained from the constraints using for n_i the defining equation (5); then, inserting them in (5) itself, one gets $n_i \equiv n_i(\alpha', \beta') = n_i(N, E)$ (see Figs. 1 and 3).

As condensation derives from the existence of the pole combined with the feature that multiplicity increases quadratically for the excited states, the continuum formula (2) is correct in predicting the collapse of the atoms in the fundamental level, but it is unable to describe what happens for $T < T_c$. The subtlety here is that the very concept of temperature, as defined in the theory of gases, cannot be straightforwardly extended to the discrete spectrum case.

Numerical calculations performed for a physical 3-dimensional "isotropic" quantum harmonic oscillator with N ranging from 10^2 to 10^{12} , made for simplicity approximating $[\psi']^{-1}$ by fixing only pole and zero,

$$n_i = \frac{1}{h_i} - \frac{6}{\pi^2} \text{ for } h_i < \pi^2/6 \text{ and } n_i = 0 \text{ for } h_i > \pi^2/6,$$

show indeed that, for E/N large, $\pi^2/6 - \alpha' \propto (E/N)^{-3}$ while $\beta' \propto (E/N)^{-4}$. The internal energy is therefore not proportional to the inverse Lagrange multiplier β'^{-1} but to the more complex expression $(\pi^2/6 - \alpha')\beta'^{-1}$. Temperature can then no longer be obtained, as in the continuum, by $T = (k_B\beta')^{-1}$ and equipartition of energy must be demonstrated. The only way to proceed is to adopt the basic definition of temperature based on entropy. In order to do so, we use Shannon's definition of entropy in terms of probabilities

$$S = -k_B \sum p_i \ln p_i$$

where we set $p_i \equiv n_i/N$, recalling that the $n_i(N, E)$'s are now known. At fixed N we thus straightforwardly obtain $S = S(E)$. Simple numerical operations finally give the temperature

$$T \equiv T(E) = \left[\frac{\partial S}{\partial E} \right]_N^{-1}.$$

Once more the function is one-to-one, and from $T = T(E)$ we can obtain $E = E(T)$ (see Fig. 4), whence the specific heat $C \equiv \frac{1}{N} \left[\frac{\partial E}{\partial T} \right]_N$ is obtained by (numerical) differentiation (see Fig. 2). Also μ , which is no longer related in a simple way to α' , can be calculated in analogous way, $\mu \equiv - \left[\frac{\partial E}{\partial N} \right]_S$, and all the results presented above are thus obtained.

It should be pointed out that the theory presented leads not only to a set of specific behaviors, but it determines as well the measurable quantities: specific heat, filling order parameter, chemical potential, etc., all of which can be experimentally measured and are related to the characteristics of the experiment (N, E, ν). To this latter effect, it should be pointed out that in the experiments the harmonic potential is usually anisotropic: extension of our results to the corresponding physical parameters is straightforward. Whether or not the features predicted theoretically are correct or not can therefore be tested by direct measurements of sufficiently high sensitivity. This feedback from the laboratory is crucial before further refinements of our analysis, such as e.g. inclusion of many body effects, is carried over.

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